Ethanol
64-17-5 | DTXSID9020584

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 4.21e-12 cm3/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 6.55e-01

Confidence level: 6.96e-01

Nearest Neighbors from the Training Set

Image not found
Ethanol
Measured: 3.27e-12
Predicted: 4.21e-12

Image not found
Isopropanol
Measured: 5.07e-12
Predicted: 5.72e-12

Image not found
1-Propanol
Measured: 5.53e-12
Predicted: 7.35e-12

Image not found
Ethyleneimine
Measured: 6.10e-12
Predicted: 9.93e-12

Image not found
1,3-Propylene oxide
Measured: 1.03e-11
Predicted: 6.49e-12